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ME469: Advection Operators: Monotonicity Through "Unwinding" and "Limiters"

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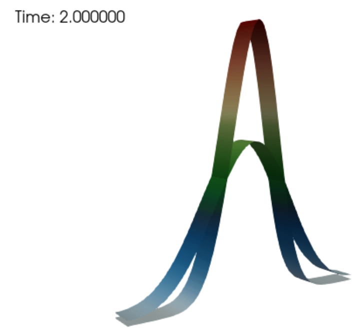
Dissipation and Dispersion Error: Review

Recall, in our modified one-dimensional advection of a passive scalar, we had two types of errors that manifested depending on the underlying numerical approach:

- Dissipative-like error:

$$\frac{\partial \phi}{\partial t} + v\frac{\partial \phi}{\partial x} - \alpha\frac{\partial^2 \phi}{\partial x^2} = 0$$

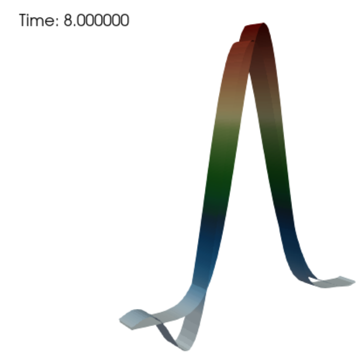
$$\phi(x,t) = e^{(-ivk-\alpha k^2)t}e^{ikx} = e^{ik(x-vt)}e^{-\alpha k^2 t}$$



- Dispersion-like error:

$$\frac{\partial \phi}{\partial t} + v\frac{\partial \phi}{\partial x} + \beta\frac{\partial^3 \phi}{\partial x^3} = 0$$

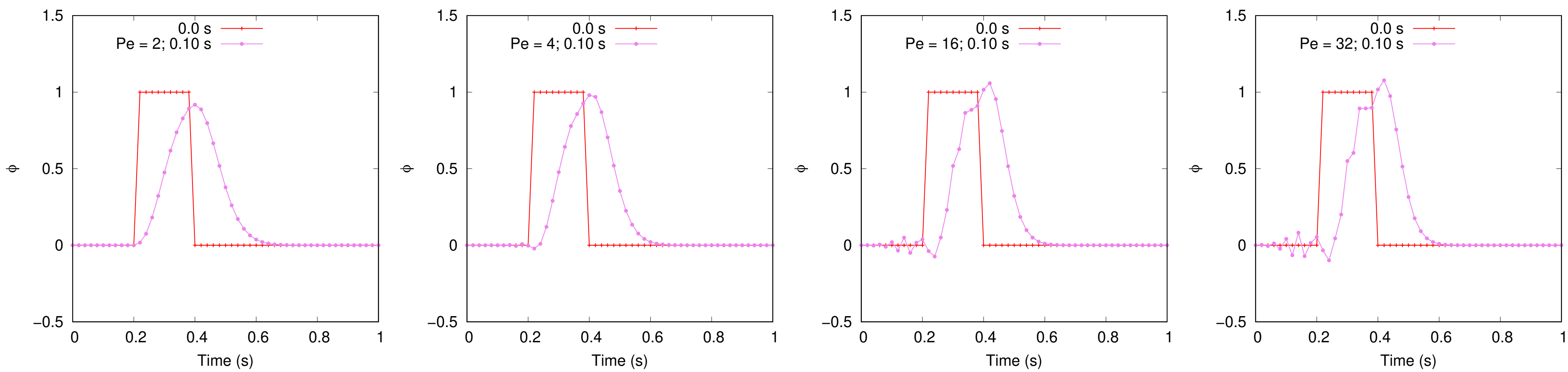
$$\phi(x,t) = e^{(-ivk+\beta ik^3)t}e^{ikx} = e^{ik[x-(v-\beta k^2)t]} = e^{ik(x-wt)}$$



Transient Advection/Diffusion: Step Function as Initial Condition Central, AKA Galerkin

Goal: Run our model equation with a variety of Peclet numbers using a step function as the initial condition

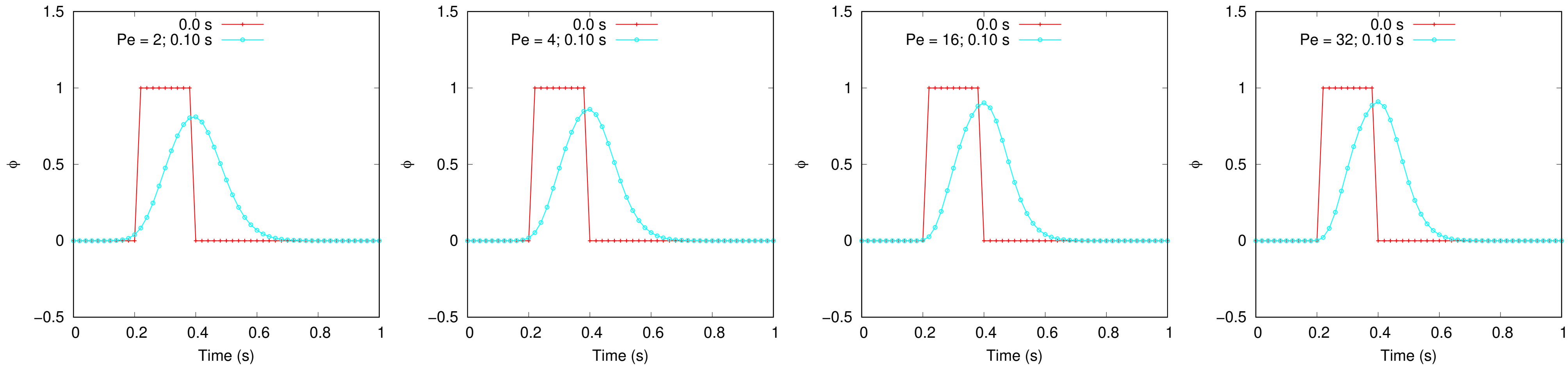
$$\int w \frac{\partial \rho u_j \phi}{\partial x_j} dV \approx \sum_{ip} (\rho u_j)_{ip} \phi_{ip} n_j dS \approx \sum_{ip} \dot{m}_{ip} \phi_{ip} \qquad \phi_{ip}^{CDS} = \sum_n N_n^{ip} \phi_n$$



Transient Advection/Diffusion: Step Function as Initial Condition First-order Upwinf

Goal: Run our model equation with a variety of Peclet numbers using a step function as the initial condition

$$\dot{m}_{ip}\phi_{ip}^{UPW} = \frac{\dot{m} + |\dot{m}|}{2}\phi_L + \frac{\dot{m} - |\dot{m}|}{2}\phi_R$$



Hybrid-Based Blending

For our general temporal advection/diffusion/source equation, can we define an improved, automatic blended approach between central and upwind?

$$\frac{\partial \rho \phi}{\partial t} + \frac{\partial \rho u_j \phi}{\partial x_j} - \frac{\partial}{\partial x_j}\left(\frac{\mu}{Sc}\frac{\partial \phi}{\partial x_j}\right) = S^{\phi}$$

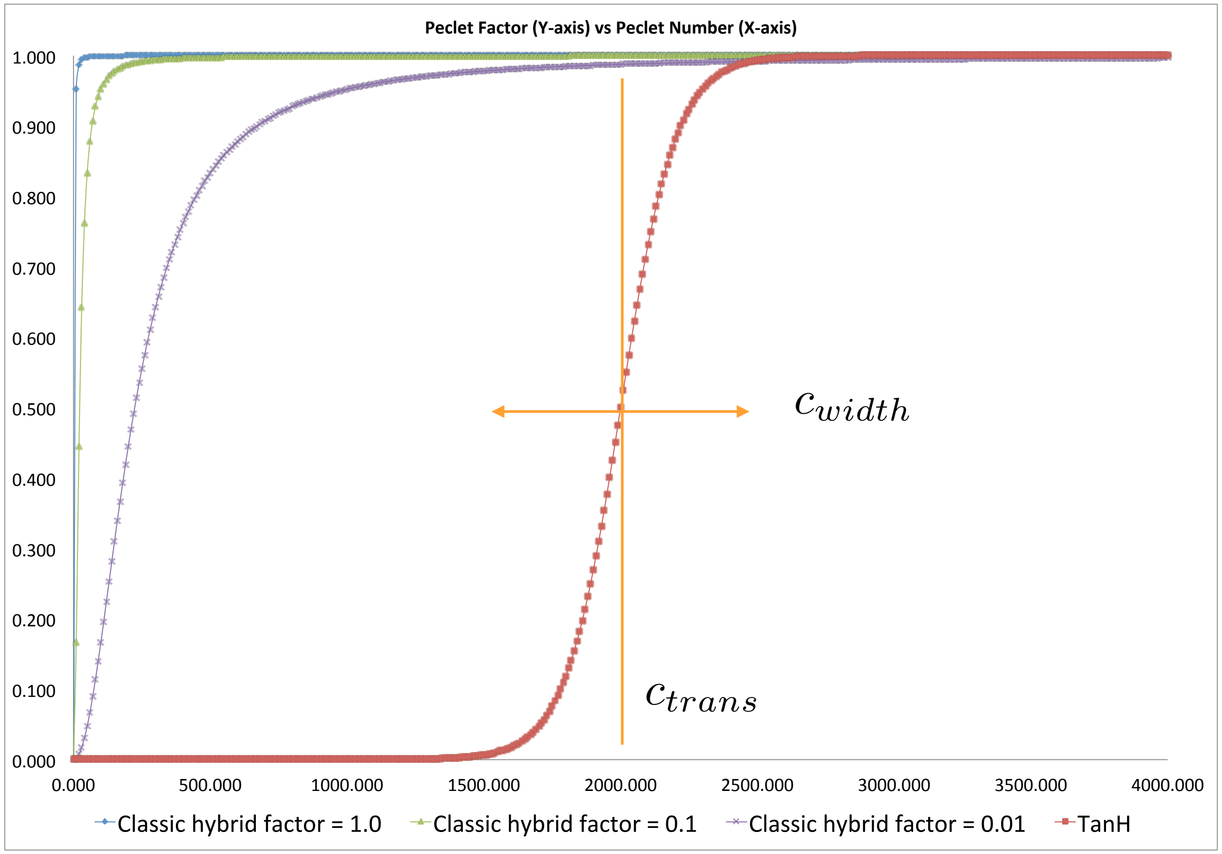
Recall, the advection operator was: $\int w \frac{\partial \rho u_j \phi}{\partial x_j} dV \approx \sum_{ip} \left(\rho u_j\right)_{ip} \phi_{ip} n_j dS \approx \sum_{ip} \dot{m}_{ip}\phi_{ip}$

With (for central, or Galerkin): $\phi_{ip}^{CDS} = \sum_{n} N_n^{ip}\phi_n$

And (for first-order upwind): $\phi_{ip}^{FOU} = \frac{\dot{m} + |\dot{m}|}{2}\phi_L + |\frac{\dot{m} - |\dot{m}|}{2}|\phi_R$

We can define a blended operator as well: $\phi_{ip} = \eta\phi^{FOU} + \left(1-\eta\right)\phi^{CDS}$

Functional form for η – Linked to Peclet number, Pe
Many ad-hoc choices, however, a common physical approach is tanh



$$Pe = \frac{\rho U L}{\mu}$$

$$\eta = \frac{1}{2}\left[1 + tanh\left(\frac{Pe - c_{trans}}{c_{width}}\right)\right]$$

- peclet_function_form:
  - velocity: tanh
  - mixture_fraction: tanh

- peclet_function_tanh_transition:
  - velocity: 5000.0
  - mixture_fraction: 2.0

- peclet_function_tanh_width:
  - velocity: 200.0
  - mixture_fraction: 4.0

Hybrid-Blending Sanity Check

Consider a simple fluids case where we have air (298.15K) flowing 1 m/s in a 1 m^3 domain

- For Pe = 2 at each element, we would require ~0.03 m resolution, or a mesh of size: ~35,000

Consider a simple fluids case where we have air (298.15K) flowing 10 m/s in a 1 m^3 domain

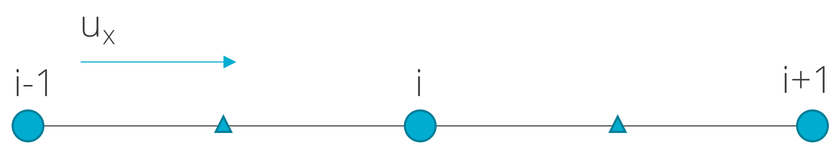
- For Pe = 2 at each element, we would require ~0.003 m resolution, or a mesh of size: ~35,000,000

- In general, this constraint results in extremely high mesh counts for most all practical flow configurations; for turbulent regimes, we would quickly revert to η = unity
- Moreover, as presented, we are blending with upwind – an operator that we have already shown to be overly diffuse and non-energy conserving

Monotonic Issues at High Pe: Simple Matrix Analysis

Consider our passive scalar concentration whose natural range (as a mass fraction) is bounded between zero and unity, here, shown as a stationary transport equation:

$$\frac{\partial \rho u_j \phi}{\partial x_j} - \frac{\partial}{\partial x_j}\left(\rho D \frac{\partial \phi}{\partial x_j}\right) = 0$$



Using our CDS and standard diffusion operator yields the following matrix system:

$$\left(\frac{\rho u}{2}\begin{bmatrix}-1 & 0 & 1\end{bmatrix} + \frac{\rho D}{\Delta x}\begin{bmatrix}-1 & 2 & -1\end{bmatrix}\right)\begin{bmatrix}\phi_{i-1} \\ \phi_i \\ \phi_{i+1}\end{bmatrix}.$$

$$a_{i,i-1} = \frac{\rho D}{\Delta x}\left(1 + \frac{Pe}{2}\right)$$

With coefficients, $a_{i,i}\phi_i = a_{i,i-1}\phi_{i-1} + a_{i,i+1}\phi_{i+1}$ and: $a_{i,i} = (a_{i,i-1} + a_{i,i+1})$

$$a_{i,i+1} = \frac{\rho D}{\Delta x}\left(1 - \frac{Pe}{2}\right)$$

Substituting: $a_{i,i-1} = a_{i,i} - a_{i,i+1}$ and defining: $\xi = \frac{a_{i,i+1}}{a_{i,i}}$

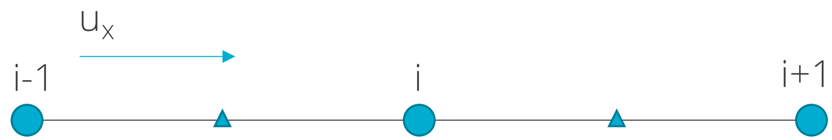
Yields: $\phi_i = \xi\phi_{i+1} + (1-\xi)\phi_{i-1}$

Positive for Pe < 2

For Pe < 2, the value of the scalar at node i is a linear combination of the neighboring values

Monotonic Issues Resolved When Using First-order Upwind

$$\frac{\partial \rho u_j \phi}{\partial x_j} - \frac{\partial}{\partial x_j}\left(\rho D \frac{\partial \phi}{\partial x_j}\right) = 0$$



$$a_{i,i-1} = \frac{\rho D}{\Delta x}(1 + Pe)$$

Positive for all Pe

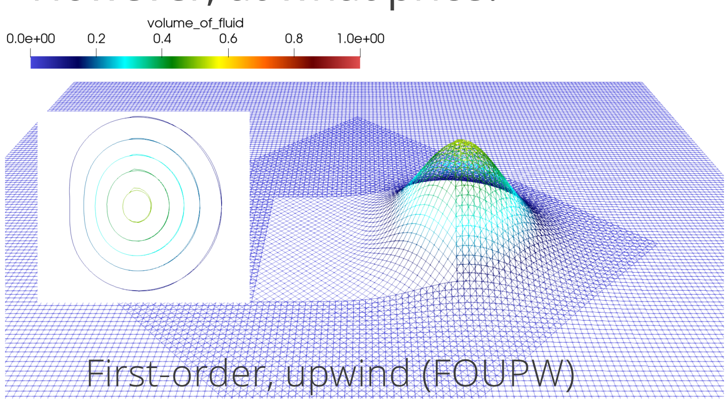
$$a_{i,i} = (a_{i,i-1} + a_{i,i+1})$$

$$a_{i,i+1} = \frac{\rho D}{\Delta x}$$

$$\left(\frac{\rho u}{2}\begin{bmatrix}-1 & 1 & 0\end{bmatrix} + \frac{\rho D}{\Delta x}\begin{bmatrix}-1 & 2 & -1\end{bmatrix}\right)\begin{bmatrix}\phi_{i-1}\\ \phi_i \\ \phi_{i+1}\end{bmatrix}$$

$$\phi_i = \xi\phi_{i+1} + (1-\xi)\phi_{i-1} \qquad \xi = \frac{a_{i,i+1}}{a_{i,i}}$$

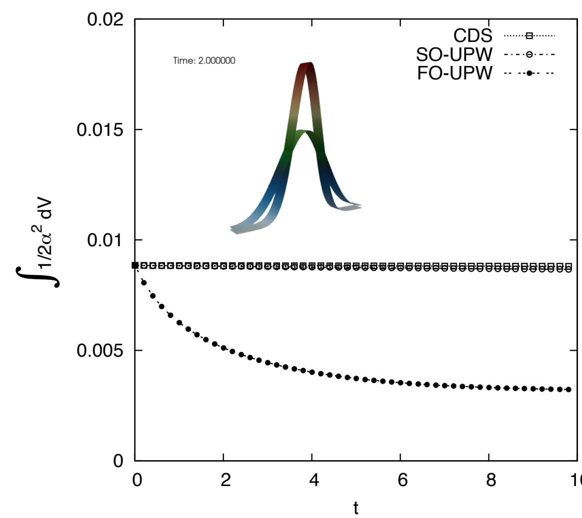
However, at what price?



First-order, upwind (FOUPW)

Fully bounded with diagonal dominance

$$\frac{\sum_{i \neq j} |a_{i,j}|}{|a_{i,i}|} \leq 1$$



Volume-of-fluid example (Domino and Horne, Renew. Ener. 2022)

Monotonic Issues at high Pe: Alternative View (Diagonal Dominance)

Define Diagonal Dominance as: $$\frac{\sum_{i\neq j}|a_{i,j}|}{|a_{i,i}|} \leq 1$$

For a monotonic operator and ease of solving the linear system, diagonal dominance is desired

In our advection/diffusion case, this is expressed as:

$$\frac{\left|\frac{\rho D}{\Delta x}\left(1-\frac{Pe}{2}\right)\right| + \left|\frac{\rho D}{\Delta x}\left(1+\frac{Pe}{2}\right)\right|}{\frac{2\rho D}{\Delta x}} \leq 1$$

Which, again, is only ensured when the Peclet number is less than two

Alternatives to First-order Upwind: Higher-order Upwind

The remaining set of slides are algebra-intensive!

- We do not intend for you to memorize these upcoming formulas, only the philosophy by which they are derived

Alternatives to First-order Upwind: Higher-order Upwind

Recall, that in the finite difference context, we could increase the upwind stencil to increase accuracy, e.g.,

Derivative	Accuracy	−8	−7	−6	−5	−4	−3	−2	−1	0
1	1								−1	1
	2							1/2	−2	3/2
	3						−1/3	3/2	−3	11/6

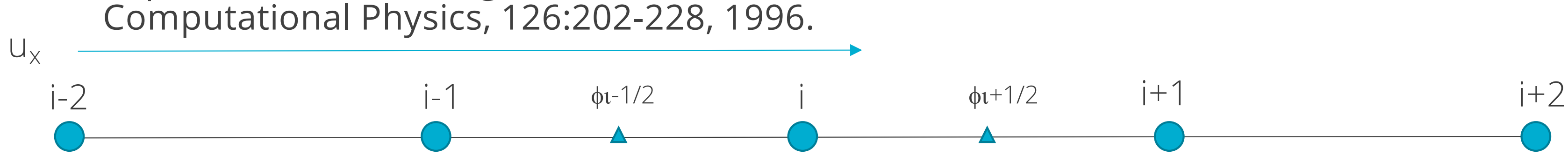
- For fluids: Varying reconstruction approaches:

Essentially Non-oscillatory (ENO)

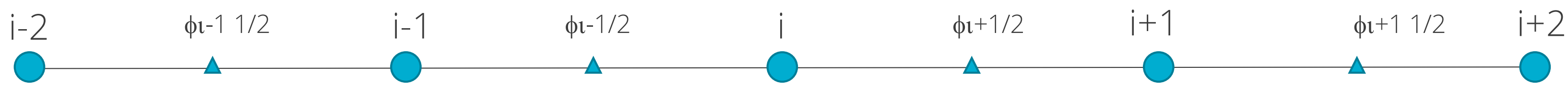
- A. Harten, B. Engquist, S. Osher and S. Chakravarthy, Uniformly high order essentially non-oscillatory schemes, III, Journal of Computational Physics, 71:231-303, 1987.

Weighted-ENO (WENO)

- 3rd-order, Liu, X., Osher, S. and Chan, T. (1994) Weighted Essentially Non-Oscillatory Schemes. Journal of Computational Physics, 115, 200-212. https://doi.org/10.1006/jcph.1994.1187
- Arbitrary-order, G. Jiang and C.-W. Shu, Efficient implementation of weighted ENO schemes, Journal of Computational Physics, 126:202-228, 1996.



ENO and WENO Concept



Define a suite of re-constructions that each provide 3rd-order accuracy:

$$\phi^{(1)}_{i+\frac{1}{2}} = \frac{1}{3}\phi_{i-2} - \frac{7}{6}\phi_{i-1} + \frac{11}{6}\phi_i \quad \phi^{(2)}_{i+\frac{1}{2}} = -\frac{1}{6}\phi_{i-1} + \frac{5}{6}\phi_i + \frac{1}{3}\phi_{i+1} \quad \phi^{(3)}_{i+\frac{1}{2}} = \frac{1}{3}\phi_i + \frac{5}{6}\phi_{i+1} - \frac{1}{6}\phi_{i+2}$$

- The above are simply defined by each of the three-point stencils, e.g.,
  - (i-2, i-1, i), (i-1, i, i+1) and (i, i+1, i+2)

We can also define a fifth-order scheme:

$$\phi_{i+\frac{1}{2}} = \frac{1}{30}\phi_{i-2} - \frac{13}{60}\phi_{i-1} + \frac{47}{60}\phi_i + \frac{9}{20}\phi_{i+1} - \frac{1}{20}\phi_{i+2}$$

- This stencil can be reconstructed based on *linear weights*, γ:

$$\gamma_1 = \frac{1}{10}, \gamma_2 = \frac{3}{5}, \gamma_3 = \frac{3}{10}$$

$$\phi_{i+\frac{1}{2}} = \gamma_1\phi^{(1)}_{i+\frac{1}{2}} + \gamma_2\phi^{(2)}_{i+\frac{1}{2}} + \gamma_3\phi^{(3)}_{i+\frac{1}{2}}$$

Or a convex-combination of weights: (sum to unity):

$$\phi_{i+\frac{1}{2}} = w_1\phi^{(1)}_{i+\frac{1}{2}} + w_2\phi^{(2)}_{i+\frac{1}{2}} + w_3\phi^{(3)}_{i+\frac{1}{2}}$$

The weights, $w_{1,2,3}$, are a function of a “smoothness” factor ($\beta_{1,2,3}$) that are dynamically selected

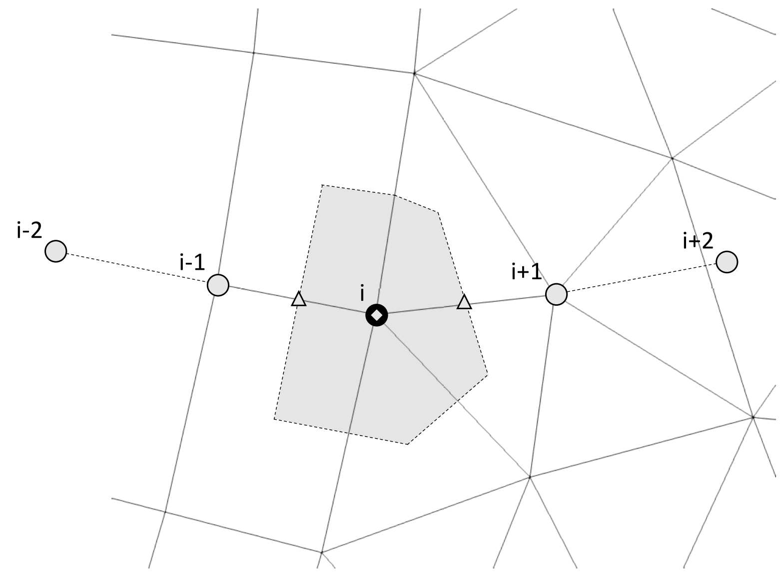
Alternatives to First-order Upwind: Higher-order Upwind – But how on an unstructured mesh?

For an unstructured setting, the former approach is not easily achieved due to the reduced stencil connectivity

- Recall, we are looping edges (as shown), or elements

- How to proceed with reconstructing data that is outside the immediate connectivity?

- Ideas?



Alternatives to First-order Upwind: Higher-order Upwind – But how on an unstructured mesh?

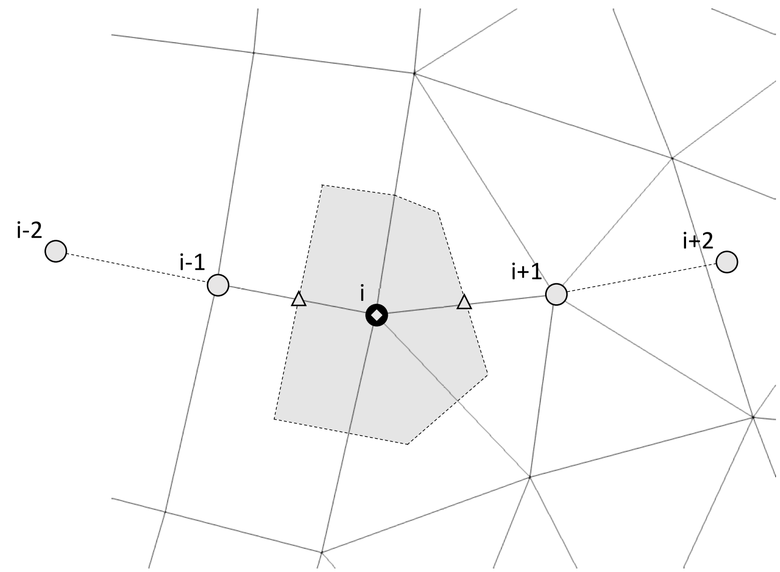
For an unstructured setting, the former approach is not easily achieved due to the reduced stencil connectivity

- Recall, we are looping edges (as shown), or elements

- How to proceed with reconstructing data that is outside the immediate connectivity?

- Ideas?

- Hint… Can we look towards the projected nodal gradient to effectively increase the stencil?



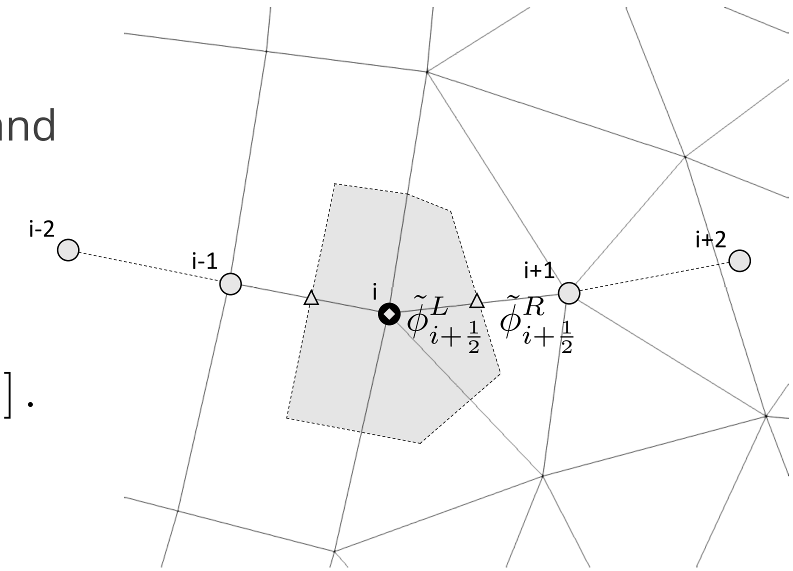
General Kappa-Method of Hirsh

Numerical Computation of Internal and External Flows, vol. 2, John Wiley & Sons, 1990

For the edge defined by the i and i+1 node, define a Left and Right state:

$$\tilde{\phi}^L_{i+\frac{1}{2}} = \phi_i + \frac{1}{4}\left[(1-\kappa)\left(\phi_i - \phi_{i-1}\right) + (1+\kappa)\left(\phi_{i+1} - \phi_i\right)\right],$$

$$\tilde{\phi}^R_{i+\frac{1}{2}} = \phi_{i+1} - \frac{1}{4}\left[(1+\kappa)\left(\phi_{i+1} - \phi_i\right) + (1-\kappa)\left(\phi_{i+2} - \phi_{i+1}\right)\right].$$



- For κ = +1, we simply revert to CDS
- For κ = -1, Second-order upwind
- For κ = 2/3, QUICK (Leonard, “A stable and accurate convective modelling procedure based on quadratic up-stream interpolation”, Comput. Methods Appl. Mech. Eng. 19 (1979) 59–98.)

Assignment: Algebra!!!

Kappa = 0 Method of Hirsh

Numerical Computation of Internal and External Flows, vol. 2, John Wiley & Sons, 1990.

- For κ = 0, recast as: (Algebra.....)

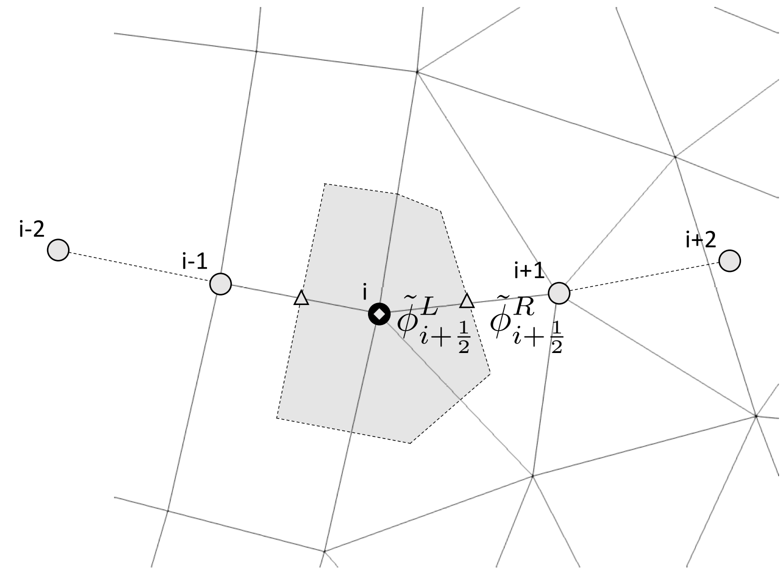
$$\tilde{\phi}^{L}_{i+\frac{1}{2}} = \phi_i + \Phi^L \Delta x^L_j G_j \phi_i,$$

$$\tilde{\phi}^{R}_{i+\frac{1}{2}} = \phi_{i+1} - \Phi^R \Delta x^R_j G_j \phi^{i+1}$$

Where,

$$\Delta x^L_j = x^{ip}_j - x^L_j,$$

$$\Delta x^R_j = x^R_j - x^{ip}_j$$



- Above, define a "limiter" function Φ^L, Φ^R that "senses" when the solution is smooth (tends towards unity) and when the solution is oscillatory (tends towards zero)
- G_j is the projected nodal gradient at each node (or cell-center) that is treated in a *deferred-correction* context, i.e., this quantity is lagged from the previous iteration
- So-called "gradient reconstruction" schemes
  - Reconstruct a higher-order stencil through extrapolation

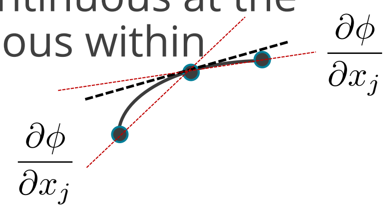
Derived by substituting κ = 0, and using the projected nodal gradient definition – or – just by noting an extrapolation using a gradient

Assignment: Algebra!!!

Projected Nodal Gradient: Refresher

- Objective: We desire a nodal variable that represents the gradient of a scalar ϕ, $G_j\phi$

- We can view the nodal gradient as continuous at the nodes/DOF location, while discontinuous within element/control volume boundaries:



Let's minimize this difference (L_2):

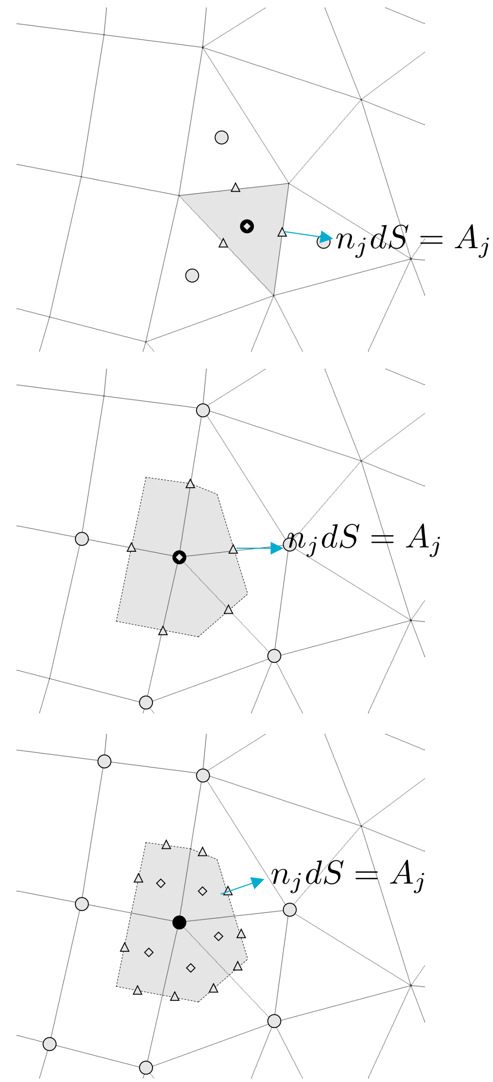
$$\int_\Omega \frac{1}{2}\left(\frac{\partial \phi}{\partial x_j} - G_j\phi\right)^2 d\Omega$$

by solving:

$$\int_\Omega w G_j \phi d\Omega = \int_\Gamma \phi n_j d\Gamma - \int_\Omega \frac{\partial w}{\partial x_j}\phi d\Omega$$

$$G_j\phi = \frac{\sum_{ip} \phi_{ip} n_j dS}{V}$$

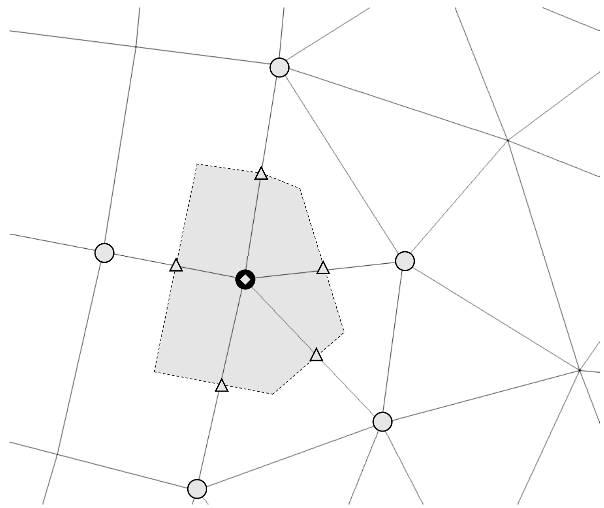
Lumped projected nodal gradient
(piecewise constant w)



Projected Nodal Gradient: Psuedo Code (Edge-based)

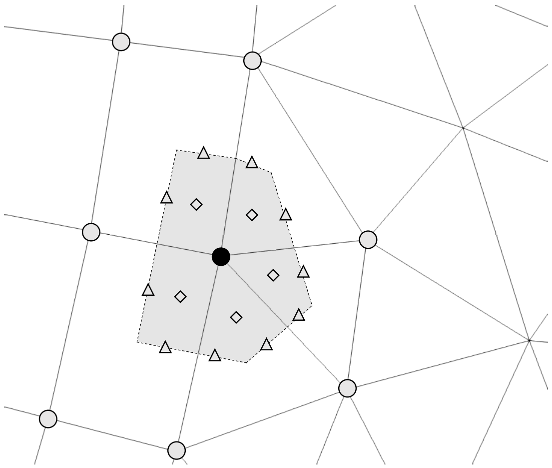
```
for ( stk::mesh::Bucket::size_type k = 0 ; k < length ; ++k ) {
     stk::mesh::Entity nodeL/nodeR = edge_node_rels[0]/edge_node_rels[1];
     const double qL = *stk::mesh::field_data( *scalarQ_, nodeL);
     const double qR = *stk::mesh::field_data( *scalarQ_, nodeR);
     const double qip = 0.5*(qL + qR);
     const double invVolL = 1.0/volL;
     const double invVolR = 1.0/volR;

     for ( int j = 0; j < nDim; ++j ) {
       const double aj = areaVector[k*nDim];
       gradQL[j] += aj*qip *invVolL;
       gradQR[j] -= aj*qip*invVolR;
     }
   }
 }
```

Rule: Area vector points from low to high global node ID

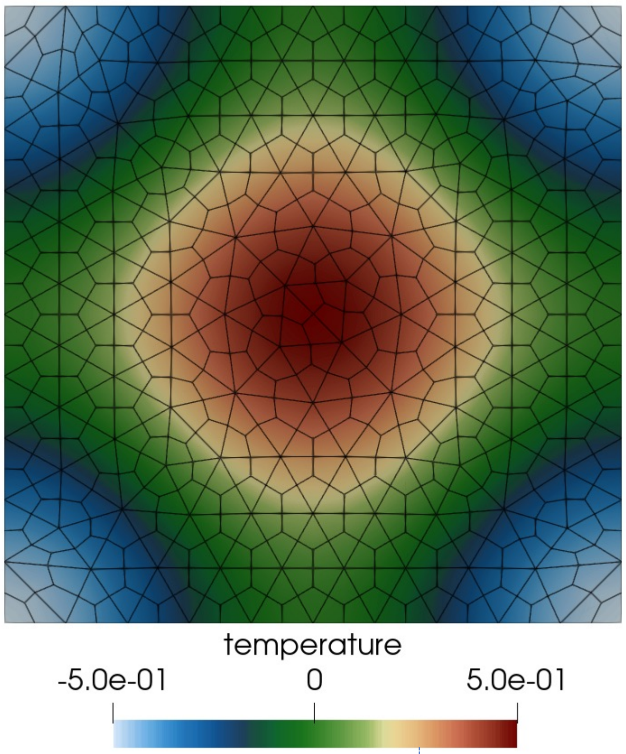


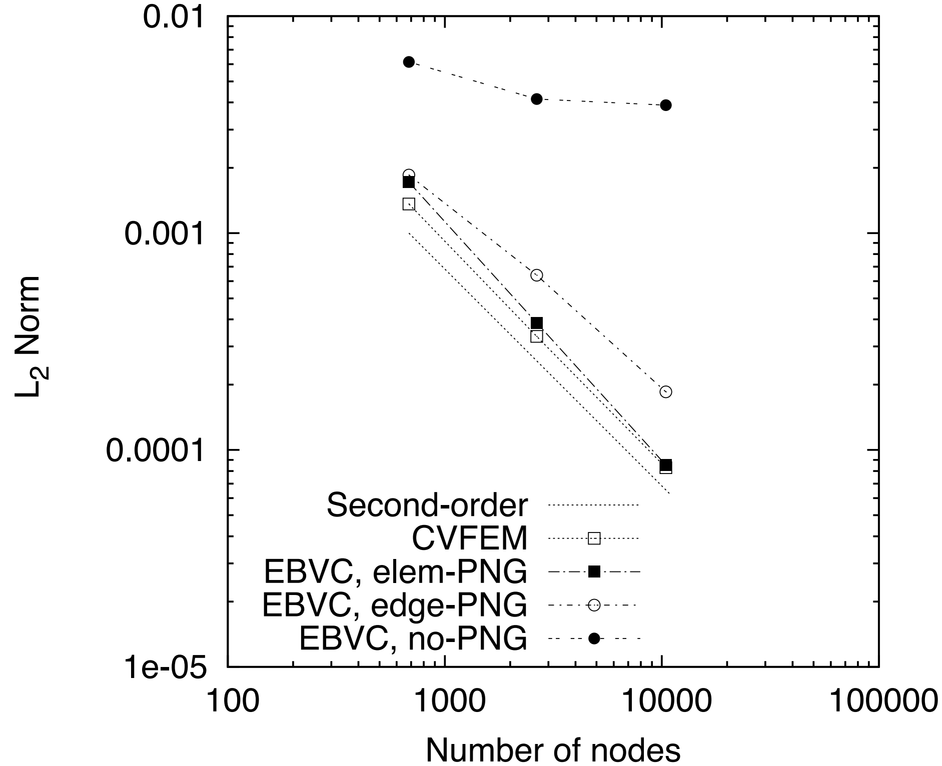
Projected Nodal Gradient: Psuedo Code (CVFEM)

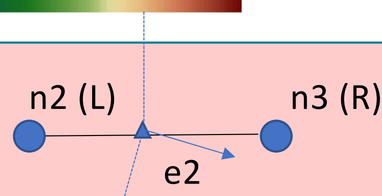
```
for ( int ip = 0; ip < numScsIp_; ++ip ) {

 // left and right nodes for this ip
 const int il = lrscv[2*ip];
 const int ir = lrscv[2*ip+1];

 double qIp = 0.0;
 const int offSet = ip*nodesPerElem_;
 for (int ic=0; ic < nodesPerElem;++ic ) {
   qIp += N[offSet+ic]*p_scalarQ[ic];
 }

 // assemble to il/ir
 for ( int j = 0; j < nDim_; ++j ) {
   double fac = qIp*areaVec[ip*nDim_+j];
   gradQL[j] += fac*inv_volL;
   gradQR[j] -= fac*inv_volR;
 }
}
```



For Instance, Verification of The Diffusion Operator



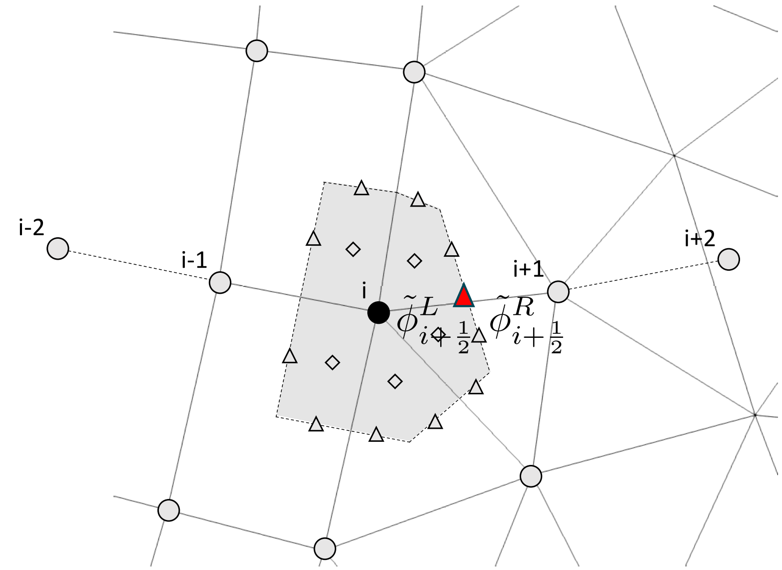




$$\frac{\partial \phi}{\partial x_j}\Big|ip = G_j^{ip}\phi + \left[(\phi_R - \phi_L) - G_l^{ip}\phi\Delta x_l\right]\frac{A_j^{ip}}{A_k\Delta x_k}$$

Kappa = 0 Method of Hirsh: CVFEM

Numerical Computation of Internal and External Flows, vol. 2, John Wiley & Sons, 1990.



- For κ = 0, recast as: (Algebra.....)

$$\tilde{\phi}^L_{i+\frac{1}{2}} = \phi_i + \Phi^L \Delta x^L_j G_j \phi_i,$$

$$\tilde{\phi}^R_{i+\frac{1}{2}} = \phi_{i+1} - \Phi^R \Delta x^R_j G_j \phi^{i+1}$$

Where,

$$\Delta x^L_j = x^{ip}_j - x^L_j,$$

$$\Delta x^R_j = x^R_j - x^{ip}_j$$

- Above, define a "limiter" function Φ^L, Φ^R that "senses" when the solution is smooth (tends towards unity) and when the solution is oscillatory (tends towards zero)
- G_j is the projected nodal gradient at each node (or cell-center) that is treated in a *deferred-correction* context, i.e., this quantity is lagged from the previous iteration
- So-called "gradient reconstruction" schemes
  - Reconstruct a higher-order stencil through extrapolation

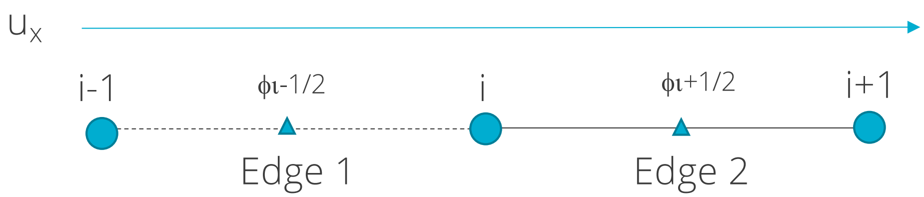
CVFEM surface integration point can be along the edge, or at the standard SCS location with modified distance verctir

Assignment: Algebra!!!

Classic Flux Limiters

Van Leer, B. (1974), "Towards the ultimate conservative difference scheme II. Monotonicity and conservation combined in a second order scheme", J. Comput. Phys., 14 (4): 361–370

- Consider our standard three-point stencil obtained by iterating edge 1 and 2



- In the above stencil, we are stressing that when iterating edge 2, we do not have information easily obtain for edge 1 (shown above as a dashed line); (speaking from an unstructured perspective)

$$\phi_{i+\frac{1}{2}} = \phi^{LOW}_{i+\frac{1}{2}} - \Phi(r_{i+\frac{1}{2}})\left(\phi^{LOW}_{i+\frac{1}{2}} - \phi^{HIGH}_{i+\frac{1}{2}}\right)$$

Monotonic upstream-centered scheme for conservation laws (MUSCL)

- Above, the “LOW” and ”HIGH” are any operators that you select, e.g.,

$$\phi^{LOW}_{i+\frac{1}{2}} = \phi_i \qquad \phi^{HIGH}_{i+\frac{1}{2}} = \frac{\phi_i + \phi_{i+1}}{2} \longrightarrow \phi_{i+\frac{1}{2}} = \phi_i + \frac{1}{2}\Phi(r_{i+\frac{1}{2}})\left(\phi_{i+1} - \phi_i\right)$$

$$r_{i+\frac{1}{2}} = \frac{(\phi_i - \phi_{i-1})}{(\phi_{i+1} - \phi_i)} \qquad (\phi_i - \phi_{i-1}) = 2G_x\phi_i\Delta x - (\phi_{i+1} - \phi_i) \qquad G_x\phi_i = \frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x}$$

Flux Limiter Definition

Sweby (1984) defined set of permissible limiter regions for the desired second-order accurate methods: A sampling of the Sweby Diagram

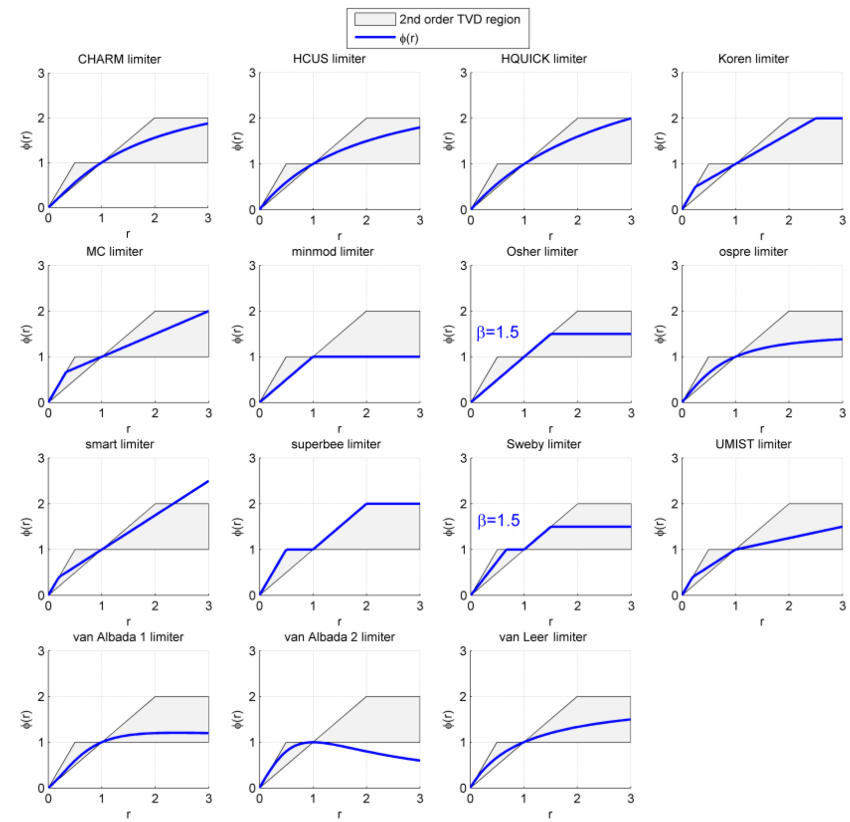
Superbee: $\Phi(r) = max[0, min[2r, 1], min[r/2]]$

Van Leer: $\Phi(r) = \dfrac{r + |r|}{1 + |r|}$

Symmetry property: $\Phi(1/r) = \dfrac{\Phi(r)}{r}$

Total Variation: $TV(\phi) = \sum_{j=1}^{N} |\phi_j - \phi_{j-1}|$

- For a monotonically increasing function, TV(ϕ) = $|\phi_1 - \phi_N|$. Note that if ϕ_1 and ϕ_N are taken constant, then, as long as the function remains monotonic the total variation is constant
- However, if TV(ϕ) increases, then this suggest oscillations in the solution have occurred



Sweby's 2nd order TVD region. Created in Matlab. Griffgruff 18:37, 11 October 2006 (UTC)

Blending Approaches to Arrive at Pseudo Higher-order Methods: Upwind and Central

Define an upwind operator now at an arbitrary integration point:

$$\begin{aligned}\phi_{ip}^{UPW} &= \alpha_{upw}\tilde{\phi}_{ip}^{L} + (1-\alpha_{upw})\,\phi_{ip}^{CDS}; \dot{m} > 0,\\ &\quad \alpha_{upw}\tilde{\phi}_{ip}^{R} + (1-\alpha_{upw})\,\phi_{ip}^{CDS}; \dot{m} < 0.\end{aligned}$$

And for a generalized CDS scheme:

$$\phi_{ip}^{GCDS} = \frac{1}{2}\left(\hat{\phi}_{ip}^{L} + \hat{\phi}_{ip}^{R}\right), \qquad \begin{aligned}\hat{\phi}_{ip}^{L} &= \alpha\tilde{\phi}_{ip}^{L} + (1-\alpha)\,\phi_{ip}^{CDS},\\ \hat{\phi}_{ip}^{R} &= \alpha\tilde{\phi}_{ip}^{R} + (1-\alpha)\,\phi_{ip}^{CDS}\end{aligned}$$

- Two new blending parameters: α_{upw} and α

The Idealized Stencil Set

With Nalu input file specifications

$i-2$	$i-1$	i	$i+1$	$i+2$	α	α_{upw}
0	$-\frac{1}{2}$	0	$+\frac{1}{2}$	0	0	n/a
$+\frac{1}{8}$	$-\frac{6}{8}$	0	$+\frac{6}{8}$	$-\frac{1}{8}$	$\frac{1}{2}$	n/a
$+\frac{1}{12}$	$-\frac{8}{12}$	0	$+\frac{8}{12}$	$-\frac{1}{12}$	$\frac{2}{3}$	n/a
$+\frac{1}{4}$	$-\frac{5}{4}$	$+\frac{3}{4}$	$+\frac{1}{4}$	0	$\dot{m} > 0$	1
0	$-\frac{1}{4}$	$-\frac{3}{4}$	$+\frac{5}{4}$	$-\frac{1}{4}$	$\dot{m} < 0$	1
$+\frac{1}{6}$	$-\frac{6}{6}$	$+\frac{3}{6}$	$+\frac{2}{6}$	0	$\dot{m} > 0$	$\frac{1}{2}$
0	$-\frac{2}{6}$	$-\frac{3}{6}$	$+\frac{6}{6}$	$-\frac{1}{6}$	$\dot{m} < 0$	$\frac{1}{2}$

- alpha_upw:
  velocity: 1.0

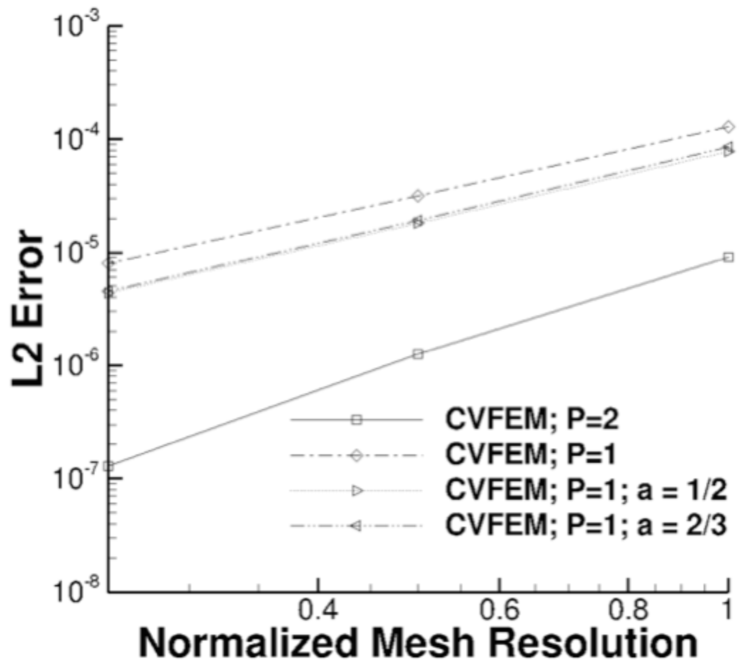
- alpha:
  velocity: 1.0

- upw_factor:
  velocity: 1.0 (zero reverts to first-order)

- limiter:
  velocity: [yes/no]

Pseudo 4th order Verification Results

Verification using Central (linear and quadratic) compared to pseudo 4th order



Lower error, however, formally second-order accurate